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28

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**J. Harper, J. Sheehy, and Bill Larson** "Isolation of Carbon Atoms in Cryogenic Solids"

**HEDM Conference Presentation**

**(Statement A)**

# Isolation of Carbon Atoms in Cryogenic Solids

J. Harper, J. A. Sheehy, and C. W. Larson

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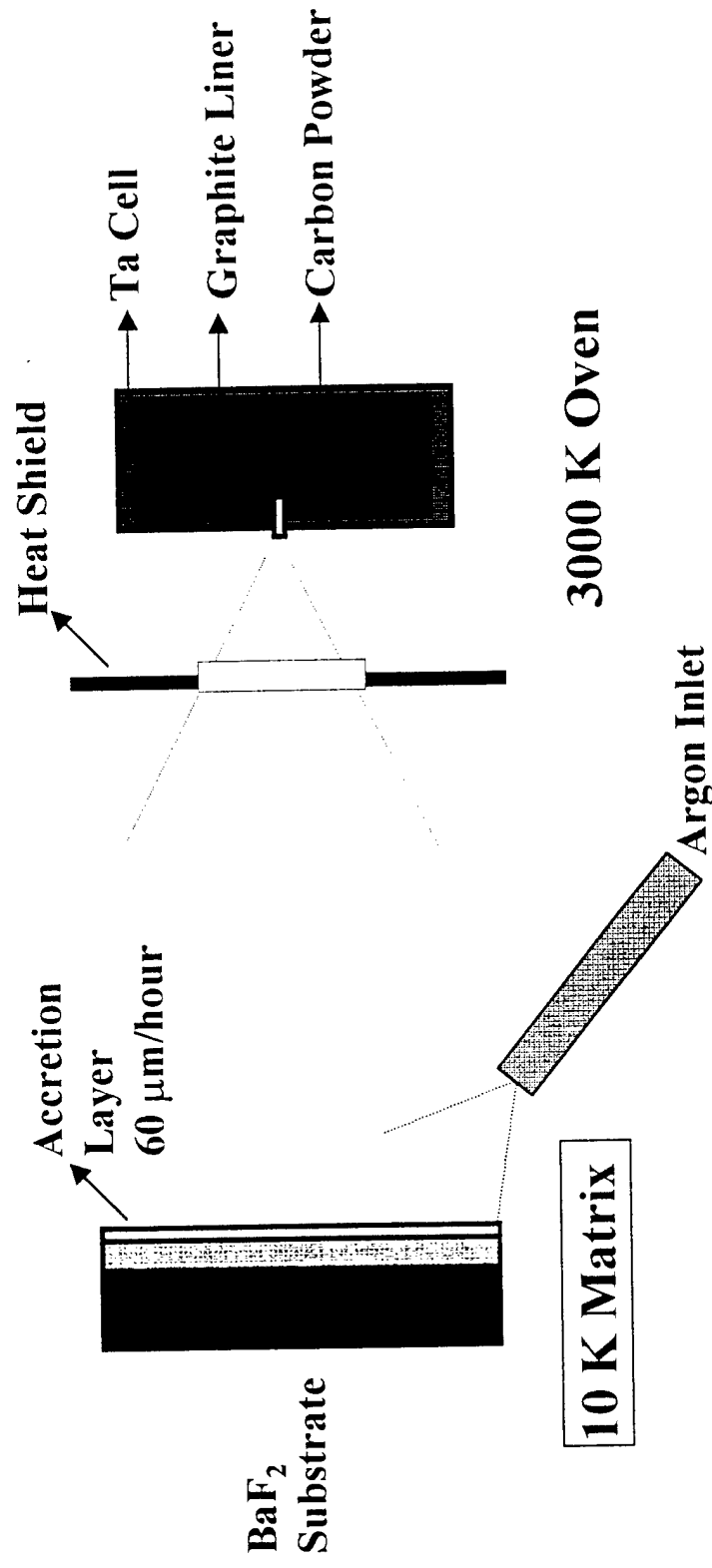
# Project Goals

- Increase production of carbon atoms from furnace source
- Prevent condensation of carbon atoms in matrix
- Develop general approach to make other HEDM propellants
- Identify new molecules through spectroscopy
- Verify IR assignments to aid in interpretation of results

**Progress toward 5% carbon atoms in solid H<sub>2</sub>**

(To yield 469s I<sub>sp</sub> propellant, compared to 389s for LOX/LH<sub>2</sub>)

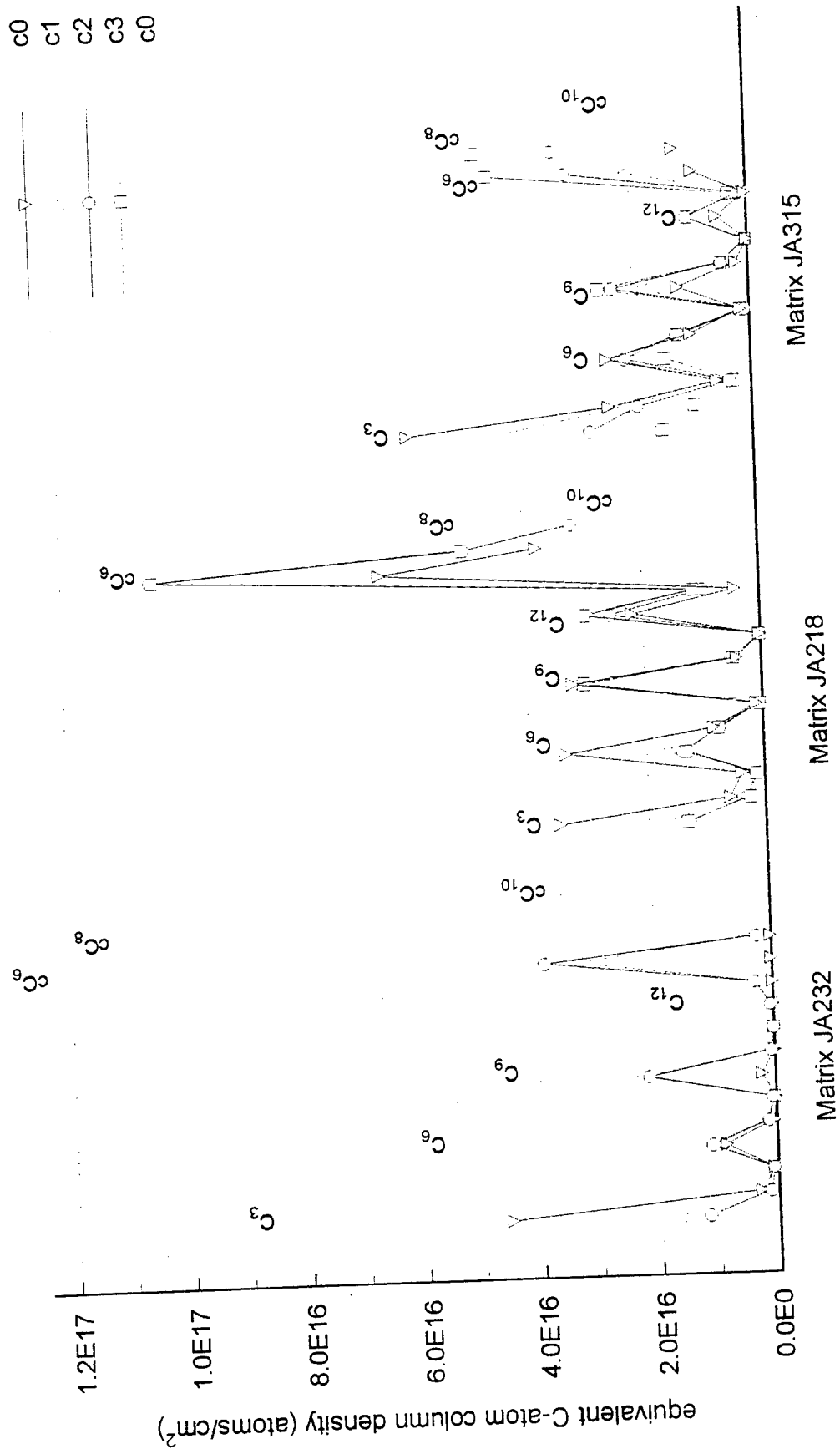
# Experiment

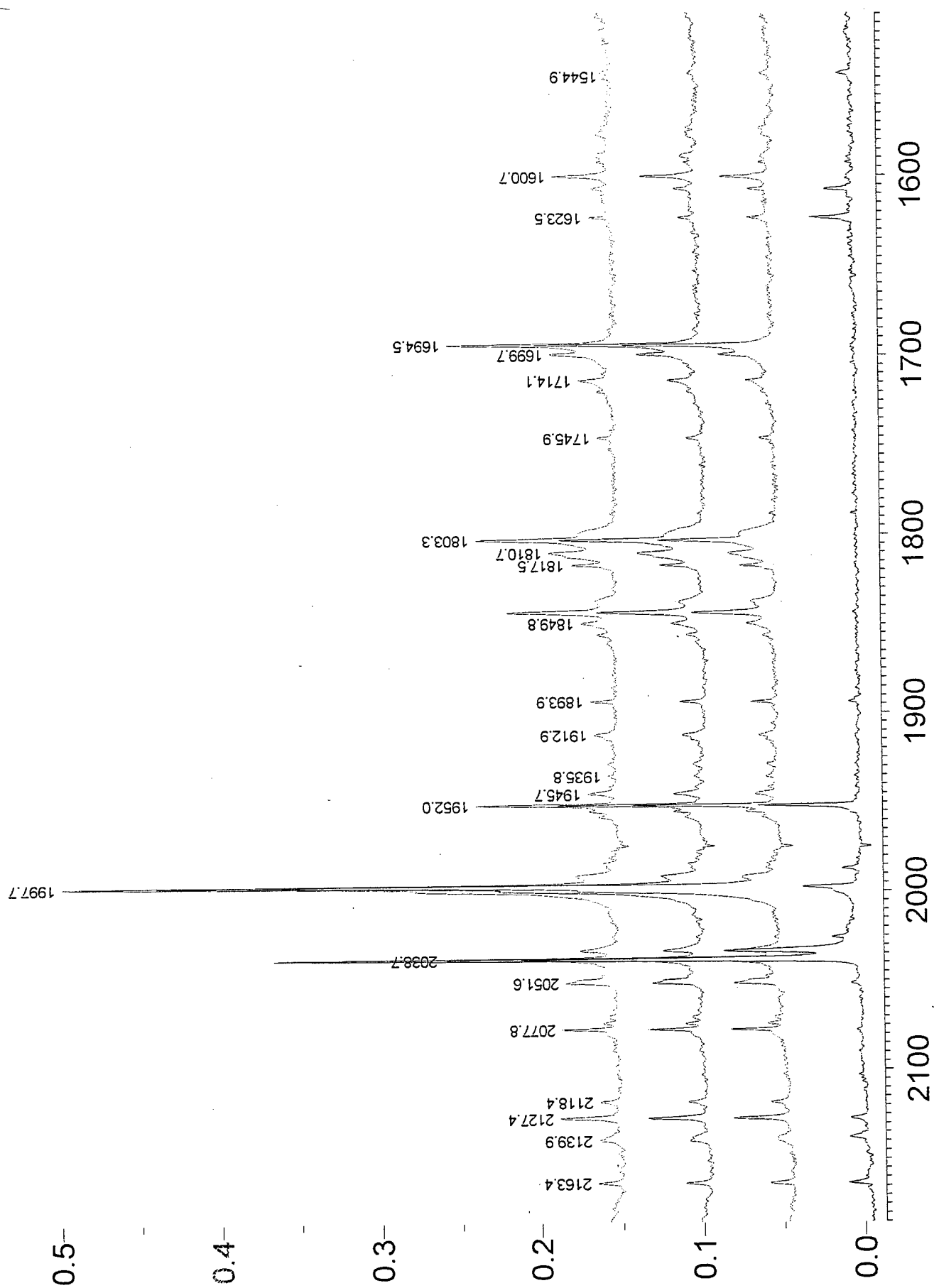


- Higher oven temperature increases carbon atom production
- Smaller iris in heat shield reduces radiative heat load on matrix from oven
- Slower argon flow rate (to a limit) increases concentration of carbon atoms
- Contaminates scavenge carbon atoms; high vacuum ( $10^{-8}$  Torr) critical

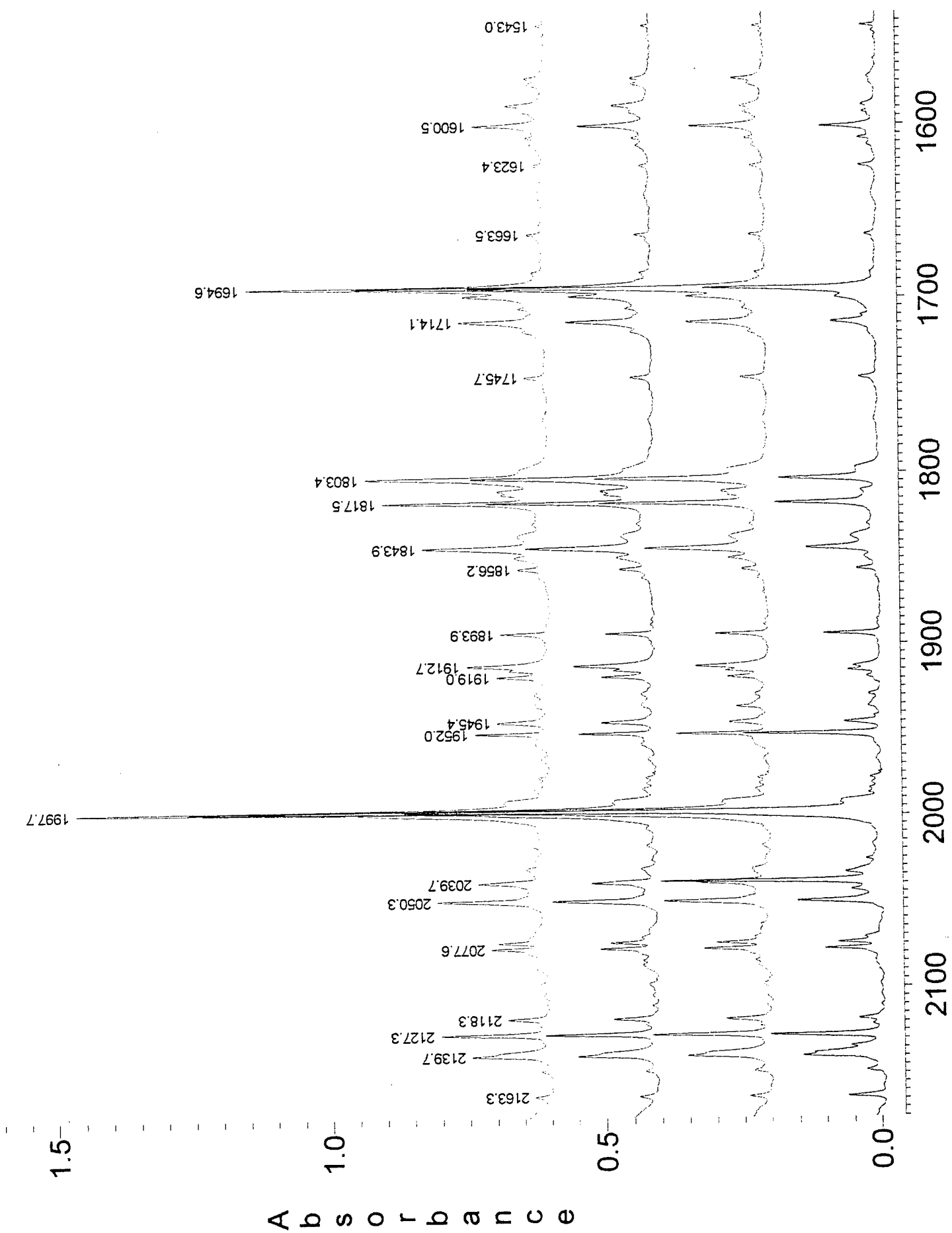
# FTIR Spectroscopy

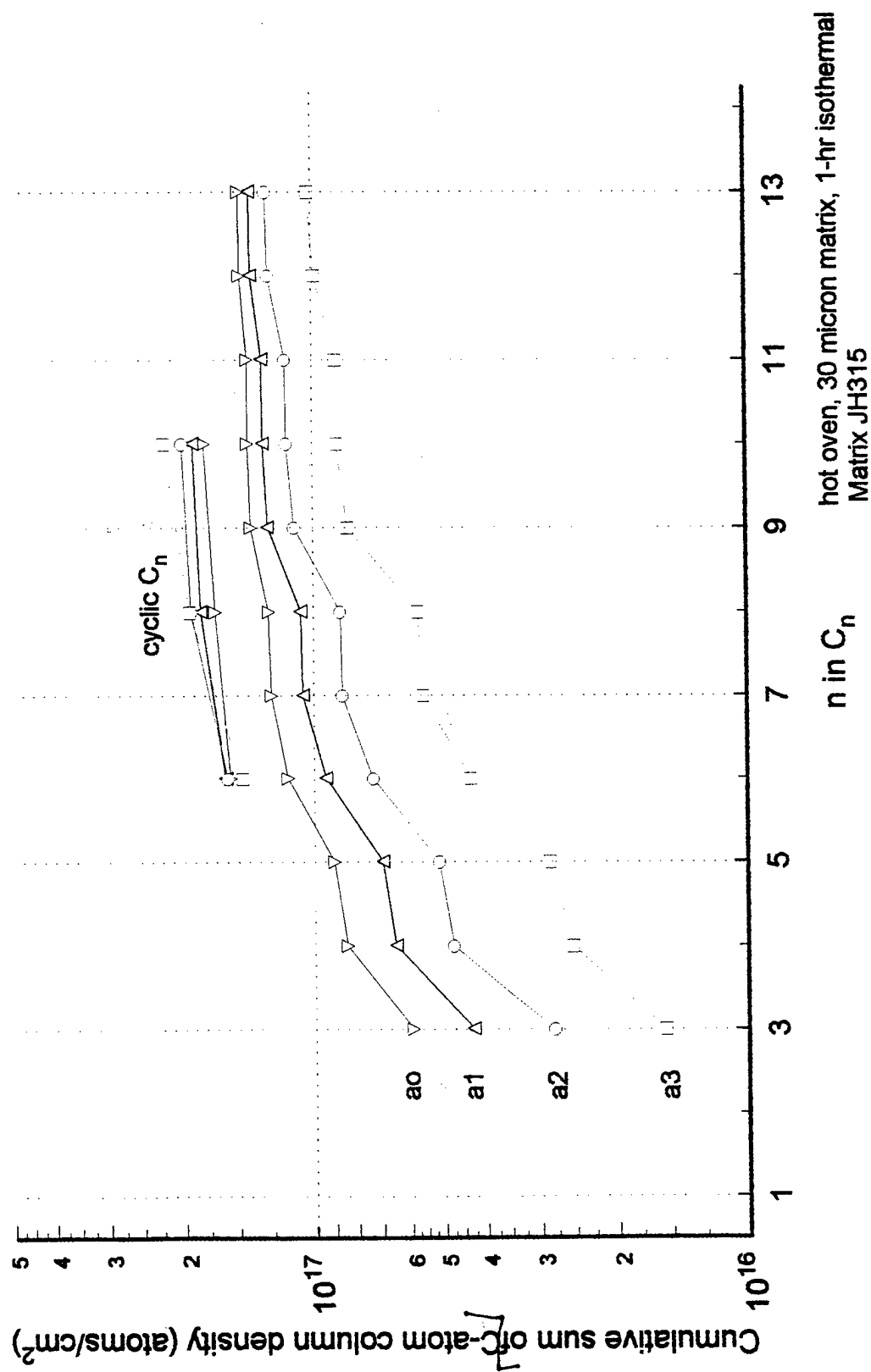
- Method for direct detection of carbon atoms unavailable
- Indirect atom detection by analysis of IR spectra taken before and after annealing of the carbon/argon matrix
  - Absolute column densities (molecules  $\text{cm}^{-2}$ ) are determined for each carbon cluster from Beer's Law.
  - Identify and track all important species that grow or disappear during annealing processes.
  - From successive cluster distributions one can calculate the quantity of carbon species that were not detected in the as-deposited matrix IR spectrum. This increase in the total equivalent carbon atom density is attributed to carbon atoms that are "invisible" to IR and were thus not accounted for in the original IR spectrum.

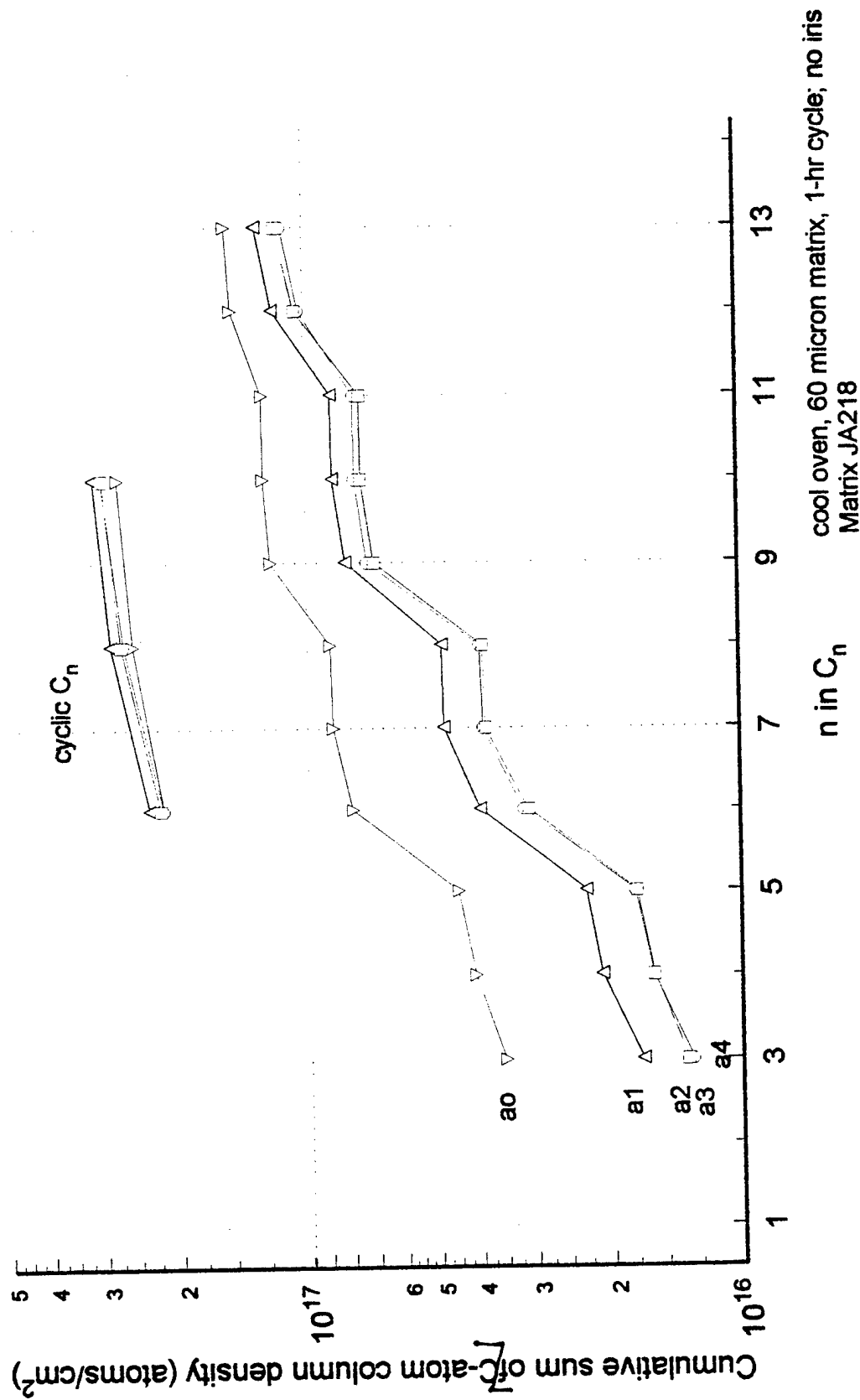










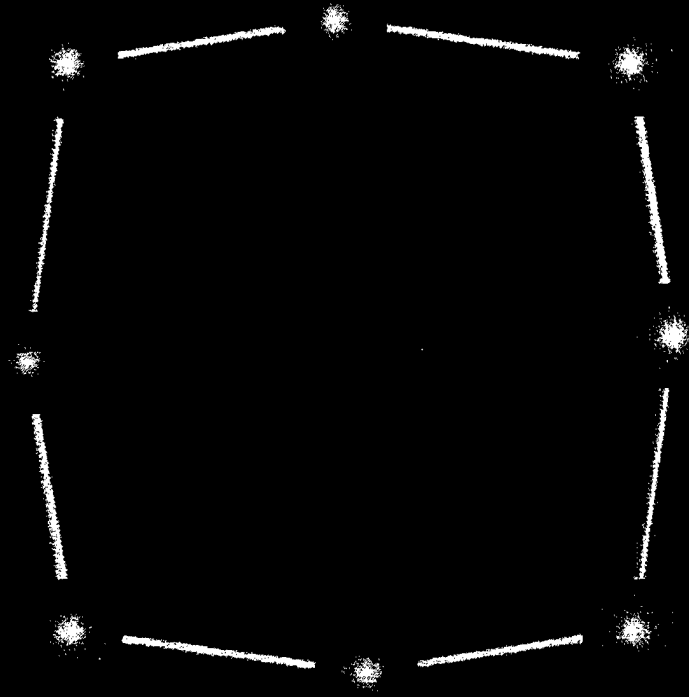


# Computational Support

- The vibrational frequencies, infrared signal intensities, absorption cross section, and isotopic frequency shifts for carbon clusters ( $c_n$   $n < 13$ ) are determined using B3LYP and CCSD(T) with cc-pVDZ and higher basis sets [6-31G\*, 6-311G, 6-311G(2d), 6-311G(2df)].
- These results aid greatly in the interpretation of infrared spectra of the matrices. Cyclic  $C_6$ , cyclic  $C_8$ , and tentatively cyclic  $C_{10}$  molecules have been identified through theoretical and experimental validation. IR frequency shifts due to matrix effects have been identified for other molecules, such as  $C_{13}$ , which are well characterized in the gas phase.

# *Cyclic $C_8$*

B3LYP/cc-pVDZ optimized structure ( $C_{4h}$  symmetry)



## Future Work

- Switch to liquid helium cryostat to perform experiments at  $4\text{K}$ . Using argon one can measure the accretion time at this temperature to compare with that from the experiments performed at  $10\text{K}$ , before moving on to depositions in  $\text{H}_2$ . A limitation to the liq. He cryostat is that the matrix in the system cannot be easily annealed.
- If results look promising, it will be worthwhile to invest in a method of direct detection of carbon atoms to use in the  $4\text{K}$  system.

# Conclusions

- Highest equivalent carbon atom concentration attained is 0.1 mol%.
- Hotter oven produces more carbon atoms
- FTIR is an effective way to derive the concentration of carbon atom equivalents in the matrices
- The temperature of the substrate is critical in preventing condensation of carbon atoms
- Unknown peaks in IR spectra have been assigned: weaker vibrational mode of C<sub>13</sub>, cyclic C<sub>8</sub>, tentatively cyclic C<sub>10</sub>
- Cyclic species dominate high density matrices